

Outer core compositions by thermoelastic properties of liquid Fe alloys

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In the outer core, many light elements, such as carbon, nitrogen, oxygen, hydrogen, sulfur, and silicon, have been proposed as possible constituents. The concentrations of these elements have long been intensely debated. Here we calculate equations of state (EoS) of pure Fe and Fe-light elements alloy liquids by means of ab initio molecular dynamics at the outer core P-T conditions and evaluate P-wave velocity based on the derived EoS, which is consistent with thermodynamic properties such as Grüneisen parameter in the similar way as Ichikawa et al. 2014. Then, we search for plausible compositions which reproduce both P-wave velocities and densities of the seismological data (PREM) (Dziewonski and Anderson, 1981) under the whole outer core conditions. Finally, we analyze the plausible compositions of the outer core, which reproduce seismological values reasonably. We found several compositions with different light elements that reproduce the seismological data to the same degree. The results also show that the influence of addition of Ni with reasonable fraction is negligibly small.

Keywords: Composition of the outer core, light elements, Ab initio molecular dynamics calculation